

Information for Contributors .....	iii
------------------------------------	-----

<b>Vapor Pressures, Critical Parameters, Boiling Points, and Triple Points of Ammonia and Trideuteroammonia .....</b>	<b>1005</b>
-----------------------------------------------------------------------------------------------------------------------	-------------

*H. W. Xiang*

A simple general corresponding-states principle has been developed to represent the vapor pressure of ammonia and trideuteroammonia from the triple point to critical point to describe the available experimental data and to extrapolate beyond their range. This work takes advantage of the adoption of the ITS-90 temperature scale and of the new critical parameters obtained from the extended corresponding-states principle. The vapor pressure data are described within their scatter in the entire temperature range. Comparisons with the available data show that the extended corresponding-states principle for vapor pressure can calculate values within 0.05% to 0.1%. The substance-dependent characteristic parameters are given, such as critical temperature, critical density, critical pressure, and acentric factor. The values of the pressures, along with their first and second derivatives as a function of temperature over the entire region from the triple point to the critical point are tabulated and recommended for scientific and practical uses.

<b>Theoretical Analysis on <math>3dnI\ J=1^e-5^e</math> Autoionizing Levels in Ca. ....</b>	<b>1013</b>
---------------------------------------------------------------------------------------------	-------------

*Dongxia Ma, Nengwu Zheng, and Jing Fan*

Previous studies on the even parity  $dnI\ j=1-5$  autoionizing levels of calcium have been critically evaluated. These levels have been studied within the framework of the Weakest Bound Electron Potential Model theory. Compared with the experimental results and the values from other theoretical methods, the present results are in concurrence with the experimental data, and showed comparative accuracy with other methods.

<b>Total, Partial, and Differential Ionization Cross Sections in Proton-Hydrogen Atom Collisions in the Energy Region of 0.1–10 keV/u. ....</b>	<b>1031</b>
-------------------------------------------------------------------------------------------------------------------------------------------------	-------------

*Lukáš Pichl, Shiyang Zou, Mineo Kimura, Izumi Murakami and Takako Kato*

Single-differential, partial, and total ionization cross sections for the proton-hydrogen atom collision system in the energy region of 100 eV/u–10 keV/u are determined by using the molecular-orbital close-coupling method within a semiclassical formalism. A critical evaluation of the existing data for the ionization process in the keV energy range is performed both for the experiment and theory.

<b>Transition Probabilities for Hydrogen-like Atoms .....</b>	<b>1059</b>
---------------------------------------------------------------	-------------

*Oliverio Jitrik and Carlos F. Bunge*

E1, M1, E2, M2, E3 and M3 transition probabilities for hydrogen-like atoms are calculated with point-nucleus Dirac eigenfunctions for  $Z=1-118$  and up to large quantum numbers  $\ell=25$  and  $n=26$ . A critical evaluation of the accuracy shows a higher reliability with respect to previous works. Tables for hydrogen containing a subset of the results are given explicitly, listing the states involved in each transition, wavelength, term energies, statistical weights, transition probabilities, oscillator strengths, and line strengths.

<b>Estimation of the Heat Capacities of Organic Liquids as a Function of Temperature Using Group Additivity. An Amendment. ....</b>	<b>1071</b>
-------------------------------------------------------------------------------------------------------------------------------------	-------------

*Milan Zábranský and Vlastimil Růžicka, Jr.*

An amendment to a second-order group additivity method for the estimation of the heat capacity of pure organic liquids as a function of temperature in the range from the melting temperature to the normal boiling temperature is reported. The present method should be more versatile and more accurate than the previous one due to the use of a larger database and an improved procedure for parameter calculation.

<b>A Unique Equation to Estimate Flash Points of Selected Pure Liquids Application to the Correction of Probably Erroneous Flash Point Values .....</b>	<b>1083</b>
---------------------------------------------------------------------------------------------------------------------------------------------------------	-------------

*Laurent Catoire and Valérie Naudet*

A simple empirical equation is presented for the estimation of closed-cup flash points for pure organic liquids. Data needed for the estimation of a flash point are the normal boiling point, the standard enthalpy of vaporization at 298.15 K of the compound, and the number of carbon atoms in the molecule. Compared to other methods, this simple equation is shown to predict accurately the flash points for a large variety of

organic compounds. Flash points of organic deuterium, organotin, organic nickel, organic phosphorus, organic boron, and organic germanium compounds can also be predicted accurately by this equation. This estimation technique has limitations concerning the polyhalogenated compounds for which the equation should be used with caution.

**Wavelengths, Energy Level Classifications, and Energy Levels for the Spectrum of Neutral Neon ..... 1113**

*E. B. Saloman and Craig J. Sansonetti*

A comprehensive critically evaluated compilation of the most accurate wavelength measurements for classified lines of Ne I has been prepared. Data from 19 sources spanning the region 256 to 54 931 Å are included. Based on this line list optimized values have been derived for the energy levels of neutral neon. In addition to the observed wavelengths, wavelengths calculated from the optimized energy levels are presented for lines that have been previously recommended for use as secondary wavelength standards.

**Recommended Liquid-Liquid Equilibrium Data  
Part 3: Alkylbenzene-Water Systems ..... 1159**

*Marian Góral, Barbara Wiśniewska-Goćłowska, and Andrzej Mączyński*

The recommended liquid-liquid equilibrium (LLE) data for 21 binary alkylbenzene-water systems have been obtained after critical evaluation of all data (392 data sets) reported in the open literature up to the middle of 2003. An equation for prediction of the alkylbenzene solubilities was developed. The predicted alkylbenzene solubilities were used for calculation of water solubility in the second liquid phase. The LLE calculations were done with the equation of state appended with a chemical term proposed by Góral.

**INDEX TO VOLUMES 31–33**

**Index of Properties and Classes of Materials—Volumes 31–33 (2002–2004) ..... 1189**

**Author Index—Volumes 31–33 (2002–2004) ..... 1193**

**JPCRD Supplements & Monographs ..... 1197**